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A method for calculating the Gibbs energies of hydrophobic effects and specific interactions of nonelectrolytes in aqueous solutions

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Abstract

The thermodynamic characteristics of hydrophobic hydration, the Gibbs energies of hydrophobic effect, were calculated. The method for calculations was based on the division of the Gibbs energy of hydration into contributions of nonspecific interactions, specific interactions between solutes and solvents (if they exist), and hydrophobic effect. In the absence of specific interactions between solutes and water, the Gibbs energy of hydrophobic effect depended linearly on the characteristic molecular volume of the solute for substances with different structures and properties. The universality of this dependence allows the suggestion to be made that it remains valid also in the presence of specific interactions. This allows the Gibbs energy of specific interactions in water to be determined for a wide range of compounds, in particular, for aliphatic alcohols. © 2008 Pleiades Publishing, Ltd.

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